



# BioCAT - The Biophysics Collaborative Access Team

A NIH-supported national user facility for structural biology of non-crystalline systems at the Advanced Photon Source

The BioCAT undulator beamline 18-ID, is a powerful and flexible instrument that can be used to address a wide range of biological problems.

## **Primary techniques supported are:**

Macromolecular small angle solution scattering  
Small angle fiber diffraction of complex biological tissues  
X-ray absorption spectroscopy

## **Macromolecular Small-angle Solution Scattering (SAS):**

SAS is an excellent technique for routine measurement of  $R_g$  (radius of gyration) and  $P_r$  (radial density distribution function) to test hypotheses concerning macromolecular conformation in solution. Our standard configurations include a 3 m camera to access a range of  $q$  from  $\sim 0.004$  to  $0.13 \text{ \AA}^{-1}$  and a 0.3 m camera for range of  $q$  from  $\sim 0.08$  to  $1.25 \text{ \AA}^{-1}$  with our 50 x 80 mm, high sensitivity CCD detector. This range of  $q$  will permit reconstruction of molecular envelopes using the spherical harmonic and dummy atom modeling approaches developed by the Svergun group. The standard sample chamber is a water-jacketed flow cell designed by Dr. Xing-Wang Fan in Prof. T. Sosnick's lab (U. Chicago). This cell takes about 100 micro-liters of sample and flows it back and forth in the beam to reduce radiation damage using a Hamilton programmable dual syringe pump. This cell design also allows mixing experiments to follow relatively slow processes (seconds-minutes). Satisfactory scattering curves can be obtained in about 1 s from 5 mg/ml cytochrome C. A complete scattering experiment can be done in less than 1/2 h depending on its complexity.

## **Small-angle fiber diffraction:**

The design features of the BioCAT beamline 18-ID and the unique source properties of the APS allow collection of fiber diffraction patterns of exceptional quality

from complex, weakly diffracting biological systems within very short exposure times. The small focal spots achievable with this instrument ( $\sim 40 \times 200$  microns) has allowed excellent discrimination of fine detail in fiber patterns from muscle, connective tissue and fibers of filamentous viruses as well as detection of weak diffraction features in the presence of large backgrounds. The low divergence of the undulator source and the independent horizontal and vertical focusing of our optics, simultaneously allows small beam spots at the sample which can be varied over a wide range. These beam sizes are very well matched to the resolution of our high sensitivity CCD detector. The high x-ray flux of this instrument ( $\sim 2.0 \times 10^{13}$  photons/s) permits dynamical experiments on these systems with potentially high time resolution. The CCD detector has very flexible binning and streak-camera modes for time-resolved experiments. The range of camera lengths we have available range from 0.18 to 5.7 m to cover a very large range of reciprocal space.

### **X-ray absorption spectroscopy:**

The BioCAT beamline has been optimized for rapid energy scanning so that scans over 1 KeV ranges can be completed in 13 s or less. The range of energies accessible with either of our two monochromators is from 3.5 to 35 keV. The small focal spots of the beam allow the use of flow techniques to reduce radiation damage, avoid freezing artifacts, and to follow kinetic phenomena at various temperatures. By acquiring data quickly, a large number of sample scans can be examined in a short period of time allowing new types of experiments to be considered. We have been developing a flexible stopped flow for both flow and rapid mixing experiments. Flow rates can range from 0.1 microliter/s to 3000 micro-liter/s. The shortest mixing time achievable is 10 ms with two syringes delivering 40 micro-liters solution through the mixer into the cell. An on-line optical monitoring system can be optionally installed to track changes in the absorption spectrum over the visible range. Temperature can be controlled from room temperature to  $-40^\circ\text{C}$ . XAS detectors include fluorescence ion chambers, large area plastic scintillator detectors, and novel BioCAT-developed analyzers to reject background. We have bent Laue analyzers suitable for studies near the Molybdenum (K-edge 20 KeV), Cadmium (K-edge 26.7 KeV) and Zinc edges (K-edge 9.66 KeV). For low and moderate energies the Multilayer Analyzer Array Detector (MAAD) provides background rejection with no count rate limits for dilute and complex systems.

### **Send us your proposals!**

Potential users are invited to contact Tom Irving ([irving@biocat1.iit.edu](mailto:irving@biocat1.iit.edu)) to discuss their needs for diffraction and scattering related experiments and Ke Zhang ([zhang@bio.aps.anl.gov](mailto:zhang@bio.aps.anl.gov)) or Grant Bunker ([bunker@biocat1.iit.edu](mailto:bunker@biocat1.iit.edu)) for XAFS related experiments. Please visit our web site at <http://www.bio.aps.anl.gov> for a description of the BioCAT facility and instructions for proposal submission.